7^{th} Quarterly Status Report **Liquid-Phase Deposition of** α **-CIS Thin Layers**

Contract # XDJ-3-30630-33

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November 12, 2004

Since the submission of our last quarterly report, we have focused on further developing the liquid-phase deposition technique in order to grow thinner layers and achieve better uniformity of the layer thickness. Apparently, the excessive thickness and roughness of the layers we deposited with the first-generation apparatus arose because the frozen material was able to lift the sliding boat.

To avoid this problem, we constructed a *second* sliding-boat apparatus. The major design change in this second construction are grooves that guide the sliding boat and keep it at constant height, such that the frozen material cannot lift it. Additionally, the new design offers better thermal contact between the melt and the thermocouple – different from the previous design, the tip of the thermocouple now resides directly beneath the substrate material.

Figure 1a shows a photograph of the reactor and the furnace. The new sliding-boat is exposed in the enlargement of Fig. 1b. Again, the construction material we utilized was graphite. Graphite is advantageous because it is not wet by the ingot material. Moreover, graphite possesses good thermal conductivity and is easily machinable. The red arrow in Fig. 1b points at the grooves guiding the sliding boat. As expected, the new construction enables the deposition of thinner layers.

From the new sliding-boat mechanism, we have deposited several layers onto the quartz–1 μm Mo–100 nm Cu substrates. (The structure of these substrates and their fabrication were described in previous reports.) We have confirmed that the stoichiometry of the newly deposited layers matches the desired stoichiometry of α -CIS. Moreover, XRD patterns revealed the dominant presence of grains with the chalcopyrite structure of α -CIS with their surface parallel to $\{112\}$ planes.

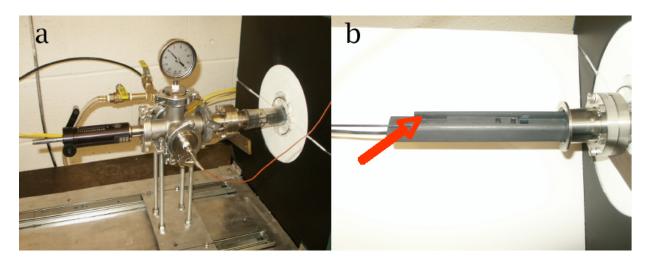


Figure 1: (a) The deposition reactor and the furnace. (b) Larger view of the new sliding-boat apparatus. The arrow points at groves guiding the boat to prevent the solidified material from pushing it up. This construction proved to be valuable for limiting the layer thickness.

In addition, to improving the sliding boat mechanism, we have made several attempts to deposit α -CIS onto (111) Si *single* crystals. The atomistic structure of the Si (111) surface has hexagonal symmetry and lattice parameters very close to those of the α -CIS (112) surface; the lattice mismatch is only \approx 6%. Based on this similarity, one would expect that α -CIS can grow *epitaxially* on (111) Si, thus as a single-crystalline layer with the same orientation as the substrate. Despite the similarity in structure, however, we have not succeeded so far in depositing α -CIS onto Si substrates.

The grain size of the layers we have obtained by liquid-phase deposition is large compared to any other deposition technique. To analyze the grain size, we have employed conventional transmission electron microscopy (TEM), and in particular dark-field imaging. This has revealed grains sizes in the range of 10 to 30 μ m in diameter. Figure 2 even exhibits *dendritic* growth of α -CIS with much larger, actually *macroscopic* grain size. Dendrites usually constitute regions with the same crystallographic orientation (although there may be small-angle grain boundaries within the dendrite). Dendritic growth can be explained by the details of heat transport through the melt and through the solid at the growth front. Since the area depicted in this micrograph is not an area that resided directly under the growth solution (ingot), but an area adjacent to it, the image provides valuable insight into the wetting and crystallization behavior of α -CIS: dendritic growth usually indicates

In addition to improving the methodology of liquid-phase deposition, we made further attempts to fabricate a working solar cell. For this purpose, CdS layers were deposited onto the liquid-phase-deposited CIS layers by chemical bath deposition. Subsequently, we deposited ZnO layers by radio-frequency sputtering. Thus far, unfortunately, the resulting devices have failed. Apparently, the problem is that the volume of the deposited layers is so large compared to the melt reservoir that secondary, metallic phases form in the upper layers of the deposit. If this hypothesis is correct, we will eliminate the problem by implementing larger reservoirs for the liquid phase. This will minimize the compositional change of the melt during the deposition process and ensure that the composition remains inside the phase field in which α -CIS is the primary

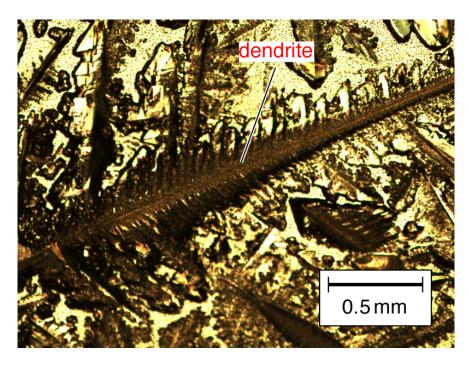


Figure 2: Optial micrograph of a layer made by liquid-phase deposition from the newly designed sliding-boat apparatus. dentric growth of α -CIS.

solidifying phase.